

Uncovering Magic Isotopes with the Power of HPC

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Where do elements come from? How does the strong force bind subatomic particles into nuclei? What can scientists understand from nuclei with unusual proton–neutron ratios? Nuclear physicists at the US Department of Energy’s (DOE’s) Oak Ridge National Laboratory (ORNL) are seeking answers to such questions with the help of powerful supercomputers.

The element tin is of particular interest to ORNL. In 2010, ORNL researchers discovered that the nucleus of a tin isotope, tin-132, was doubly “magic.” Isotopes are deemed magic when they have nucleons (positively charged proton particles or neutrally charged neutron particles) that complete a shell within the nucleus, making the magic isotopes much more strongly bound than those that are not magic. Isotopes with 2, 8, 20, 28, 50, 82, or 126 neutrons or protons are considered magic. A doubly magic isotope has two of these special numbers—one that describes its number of protons and one that describes its number of neutrons. Tin-132, for example, has 50 protons and 82 neutrons.

The discovery of new magic isotopes can significantly affect the chart of nuclides, a table that orders the radioactive behaviors of isotopes. Because magic isotopes are more strongly bound, their structure impacts entire regions of the chart of nuclides and the limit of how many nuclei can exist.

AN ISOTOPE WITH UNIQUE PROPERTIES

Now a team of nuclear physicists at ORNL and collaborators have simulated tin-100, an isotope that researchers have long sought to understand. Tin-100 is not only doubly magic but also possesses the same number of protons and neutrons (50 each). On the chart of nuclides, tin-100 exists in a region where, if a proton is added, a proton is ejected from the nucleus in the same way that someone might be eliminated from a game of musical chairs.

Using the Cray XK7 Titan supercomputer at the Oak Ridge Leadership Computing Facility (OLCF), a DOE Office of Science User Facility at ORNL, the team computed the structure of the tin-100 nucleus (and its neighbors), a configuration consisting of 100 strongly interacting particles, and determined that the isotope does, in fact, have a doubly magic nature. The team

collaborated with researchers at TRIUMF in Canada, the Institut für Kernphysik at TU Darmstadt in Germany, and Reed College in Oregon to complete the simulations (see Figure 1).

Scientists have previously computed tin-100—but from the nucleus strontium-88 instead. This distinction is crucial because previous simulations have consisted of only 12 particles, or “bodies,” rather than 100. The team at ORNL is the first to solve a problem where every single body was active, meaning there were 100 strongly interacting particles to account for.

“We are the first to provide a realistic solution of a nuclear 100-body problem starting from forces that describe how two and three nucleons interact with each other,” said Titus Morris, a postdoctoral researcher in ORNL’s Quantum Information Group. “There were so many strongly interacting particles, we really needed a supercomputer so we could describe them as exactly as possible.”

Heavy elements tend to have more neutrons to keep the charged protons apart and lower the energy of the nucleus. Therefore, although tin-100’s equal number of protons and neutrons makes it neutron-deficient and weakly bound, the nuclear force is strong enough to bind it. The results led scientists closer to an understanding of astrophysical phenomena and the elements’ origins. They also provided a look into some of the most fundamental aspects of subatomic particles, which could inform larger simulations of even heavier nuclei.

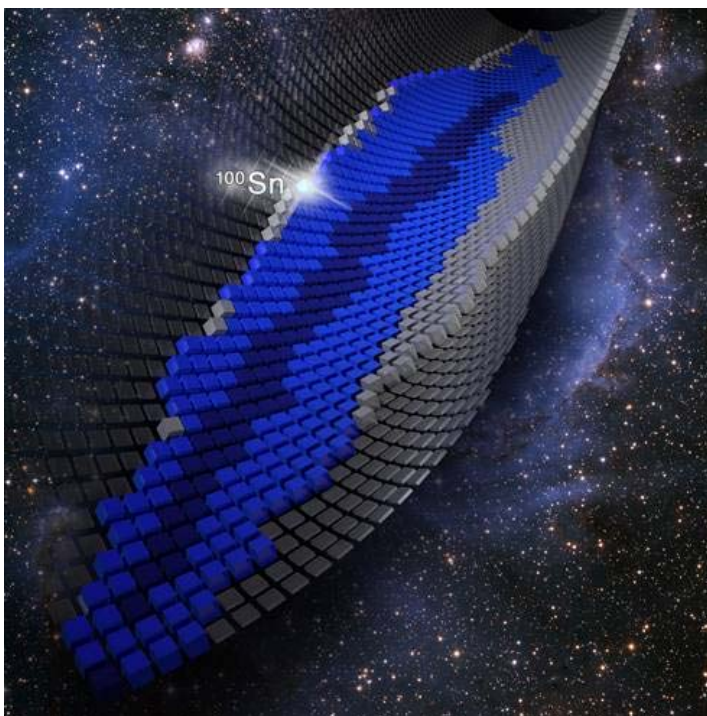


Figure 1. 3D rendered image of tin-100 in the nuclear structure and decay chart. Tin-100 sits in the region where alpha decay is a competing mechanism to beta decay. Image: Andrew Sproles, Oak Ridge National Laboratory.

HEAVY NUCLEI, HEAVY COMPUTATIONS

On the basis of early calculations used to anticipate particle behavior, the team modeled the tin-100 nucleus on Titan under the OLCF’s Innovative and Novel Computational Impact on Theory and Experiment, or INCITE program, to find out what is really happening inside this heavy exotic isotope.

“We already know how the nuclear force works in light systems,” said Gaute Hagen, a researcher at ORNL. “But we were able to link this much heavier, 100-body system to nuclear

forces that were only known well enough in very light nuclei. So it's a tremendous extrapolation and works surprisingly well at this scale."

The findings show how scientists can use high-performance computing (HPC) resources to uncover crucial details about atomic nuclei.

"Our simulations of tin-100 can give us a base for studying interactions in even heavier nuclei," said Thomas Papenbrock, a researcher at the University of Tennessee and ORNL. Because the simulations consisted of 100 strongly interacting nucleons, the project demanded HPC resources. Each of the team's many runs used up to 3,000 of Titan's nodes, and the project consumed tens of millions of core hours.

The ORNL team used the NUCCOR code, a nuclear physics application that allows scientists to recreate the structure and reactions of atomic nuclei, to complete the simulations. NUCCOR is one of 13 codes selected for the OLCF's Center for Accelerated Application Readiness (CAAR) project. With the recent arrival of the OLCF's new leadership-class supercomputer, the IBM AC922 Summit, CAAR teams are continuing to optimize their codes to ensure their performance on the system when it is fully available to users in 2019.

A NEW MAGIC NUMBER

Hagen, Morris, and Gustav Jansen, a computational scientist in the Scientific Computing Group at the OLCF, also recently used NUCCOR on Titan to decipher how well a given particle interaction predicts the energy and the radius of a nucleus.

The team gathered observable data—such as the charge radius, the amount of energy required to remove nucleons, or the effect on nuclei when more nucleons are added—for carbon isotopes and also performed new measurements. The team studied the chain of isotopes up to even more neutron-rich isotopes and discovered that the proton number six is also magic. This magicity, the quality of carrying a magic number of protons, prevailed through all the neutron-rich carbon isotopes, confirming the results of previous experiments.

With the help of Titan, the team was able to use different nuclear forces to model these isotopes. For this modeling, the researchers used effective field theory (EFT), a theory that allows for the inclusion of the physics that occur at the desired scales while ignoring those that occur outside of this range. EFT is rooted in quantum chromodynamics, a theory that describes the interactions between the fundamental particles. The team simulated dozens of interactions to see which ones better described the energy and radius of a given isotope. The data from these kinds of simulations can lead researchers to regions on the chart of nuclides that could contain yet-to-be-discovered magic numbers of nucleons.

"There is a big family of interactions that describes how we think neutrons and protons interact," Morris said. "They are a little bit different from each other, and we aren't sure how to make the process of describing these completely robust. Using resources like Titan, we can gain new insights into these interactions."

DELVING INTO THE UNKNOWN

The findings from these studies can help researchers better understand the strong force that binds protons and neutrons into nuclei. They can also allow researchers to study heavier elements much more readily.

"If we understand tin-100, then we understand all the nuclei that are a little bit heavier," Papenbrock said. "We can subtract 100 particles, because they don't react much. That's why this nucleus is important."

The research can also lead to an understanding about where elements heavier than iron are formed. A process called rapid proton capture occurs in space when many hot protons are continually "captured" by an element, leading to the formation of heavy elements. The process is unique because it occurs on the proton-rich side of the chart of nuclides rather than the neutron-rich side.

A decay process called alpha decay typically stabilizes heavy nuclei by emitting a helium nucleus. Tin-100, though, exists in a region on the chart where alpha decay competes with a process called beta decay, which occurs when protons simply decay into neutrons. The reason for this anomaly is that tin-100 has a much lower neutron-to-proton ratio than is typical of heavy elements. In fact, no other heavier doubly magic nucleus has an equal number of protons and neutrons.

“People have measured the mass of tin-100, so they know it exists,” Papenbrock said. “And they’ve measured its beta decay and know it’s one of the shortest-lived isotopes with a strong beta decay. But they don’t know its structure, and therefore our results will be useful to the experimentalists who will determine some of these unknowns.”

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